Chapter 4: Calculations
Knowledge organiser

Formula mass

Every substance has a **formula mass**, M_r.

formula mass M_r = sum (relative atomic mass of all the atoms in the formula)

Avogadro's constant (HT only)

One mole of a substance contains 6.02×10^{23} atoms, ions, or molecules. This is **Avogadro's constant**.

One mole of a substance has the same mass as the M_r of the substance. For example, the M_r (H_2O) = 18, so 18 g of water molecules contains 6.02×10^{23} molecules, and is called one mole of water.

You can write this as: moles = $\dfrac{mass}{M_r}$

Theoretical yield

The **theoretical yield** of a chemical reaction is the mass of a product that you expect to be produced.

Even though no atoms are gained or lost during a chemical reaction, it is not always possible to obtain the theoretical yield because

- some of the product can be lost when it is separated from the reaction mixture
- there can be unexpected side reactions between reactants that produce different products
- the reaction may be reversible.

Percentage yield

The **yield** is the amount of product that you actually get in a chemical reaction.

Percentage yield is the actual yield as a proportion of the theoretical yield:

percentage yield = $\dfrac{actual\ yield}{theoretical\ yield} \times 100$

Atom economy

The **atom economy** of a reaction tells you the proportion of atoms that you started with that are part of *useful* products.

High atom economies are more sustainable, as they mean fewer atoms are being wasted in products that are not useful.

The percentage atom economy is calculated by:

atom economy = $\dfrac{M_r\ of\ useful\ product}{M_r\ of\ all\ products} \times 100$

Using balanced equations (HT only)

In a balanced symbol equation the sum of the M_r of the reactants equals the sum of the M_r of the products.

If you are asked what mass of a product will be formed from a given mass of a specific reactant, you can use the steps below to calculate the result.

1 balance the symbol equation
2 calculate moles of the substance with a known mass using moles = $\dfrac{mass}{M_r}$
3 using the balanced symbol equation, work out the number of moles of the unknown substance
4 calculate the mass of the unknown substance using mass = moles × M_r

If you are asked to balance an equation, you can use the steps below to work out the answer.

1 work out M_r of all the substances
2 calculate the number of moles of each substance in the reaction using moles = $\dfrac{mass}{M_r}$
3 convert to a whole number ratio
4 balance the symbol equation

Concentration

Concentration is the amount of solute in a volume of solvent.

The unit of concentration is g/dm^3. Concentration can be calculated using:

concentration (g/dm^3) = $\dfrac{mass\ (g)}{volume\ (dm^3)}$

Sometimes volume is measured in cm^3:

volume (dm^3) = $\dfrac{volume\ (cm^3)}{1000}$

- lots of solute in little solution = high concentration
- little solute in lots of solution = low concentration

Moles of gases (HT only)

At any given temperature and pressure, the same number of moles of a gas will occupy the same volume.

At room temperature (25 °C) and pressure (1 atm), one mole of *any* gas will occupy 24 dm^3.

To calculate the number of moles of a gas:

moles of a gas = $\dfrac{volume\ (dm^3)}{24\ dm^3}$

or

moles of a gas = $\dfrac{volume\ (cm^3)}{24\,000\ cm^3}$

Concentration in mol/dm³

Concentration can also be measured in mol/dm^3.

concentration of solution (mol/dm^3) = $\dfrac{number\ of\ moles\ of\ solute}{volume\ of\ solution\ (dm^3)}$

You can use this formula and mass = moles × M_r to calculate the mass of solute dissolved in a solution.
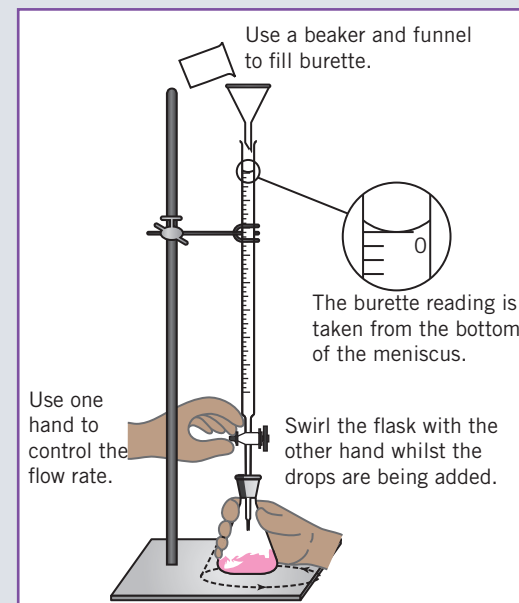
- The greater the mass of solute in solution, the greater the number of moles of solute, and therefore the greater the concentration.
- If the same number moles of solute is dissolved in a smaller volume of solution, the concentration will be greater.

> mol is a the unit of moles

Calculating concentration

To calculate the concentration of the unknown solution (the solution in the conical flask):

1 Write a balanced symbol equation for the reaction.
2 Calculate the moles used from the known solution using:

moles = concentration (mol/dm^3) × volume (dm^3)

3 Use the ratio from the balanced symbol equation to deduce the number of moles present in the unknown solution.
4 Calculate the concentration of the unknown solution using:

concentration (mol/dm^3) = $\dfrac{moles}{volume\ (dm^3)}$

Excess and limiting reactants (HT only)

In a chemical reaction between two or more reactants, often one of the reactants will run out before the others. You then have some of the other reactants left over. The reactant that is left over is in **excess**. The reactant that runs out is the **limiting reactant**.

To work out which reactants are in excess and which is the limiting reactant, you need to:

1 write the balanced symbol equation for the reaction
2 pick one of the reactants and its quantity as given in the question
3 use the ratio of the reactants in the balanced equation to see how much of the other reactant you need
4 compare this value to the quantity given in the question
5 determine which reactant is in excess and which is limiting.

Titration

Titration is an experimental technique to work out the concentration of an unknown solution in the reaction between an acid and an alkali.

1 Use a pipette to extract a known volume of the solution with an unknown concentration. A pipette measures a fixed volume only.
2 Add the solution of unknown concentration to a conical flask and put the conical flask on a white tile.
3 Add a few drops of a suitable indicator to the conical flask.
4 Add the other solution with a known concentration to the burette.
5 Carry out a rough titration to find out approximately what volume of solution in the burette needs to be added to the solution in the conical flask. Add the solution from the burette to the solution in the conical flask 1 cm^3 at a time until the end point is reached.
6 The end point is when the indicator just changes colour.
7 Record the volume of the end point as your rough value.
8 Now repeat steps 1–7, but as you approach the end point add the solution from the burette drop-by-drop. Swirl the conical flask in between drops.
9 Record the volume of the end point.

Use a beaker and funnel to fill burette.

The burette reading is taken from the bottom of the meniscus.

Use one hand to control the flow rate.

Swirl the flask with the other hand whilst the drops are being added.